OAK RIDGE National Laboratory

SAMMY Modernization and Advances in Nuclear Data Evaluation Methods

Goran Arbanas, Dorothea Wiarda, Andrew Holcomb, Marco Pigni, Vlad Sobes, Chris Chapman (ORNL), Jesse Brown (RPI)

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Outline

- SAMMY history and overview of features
- SAMMY modernization review and update
  - SAMMY 8.1 release
  - Modernization strategy
  - Example: Coulomb functions
  - SAMMY 8.2 features (early 2019)
- SAMMY future directions
  - Simultaneous optimization of thermal and resolved R-matrix
  - Bayesian generalized data optimization for defective models
  - Direct capture parameterization by imaginary channel radius
  - Generalized Reich-Moore approximation and its Brune transform
- Summary and outlook

History of SAMMY

- Developed by Dr. Nancy Larson since 1970s
- Includes SAMMY + 25 auxiliary codes (e.g., SAMRML shared by AMPX and NJOY)
- Architecture is a large Fortran (77) container array for memory management
- Includes 185 multi-step test cases + 10 tutorial examples
- Comprehensive documentation available at: http://info.ornl.gov/sites/publications/files/Pub13056.pdf
- Employed for resolved resonance evaluations in ENDF
- SAMMY 8.1 distributed via RSICC https://rsicc.ornl.gov/

SAMMY capabilities

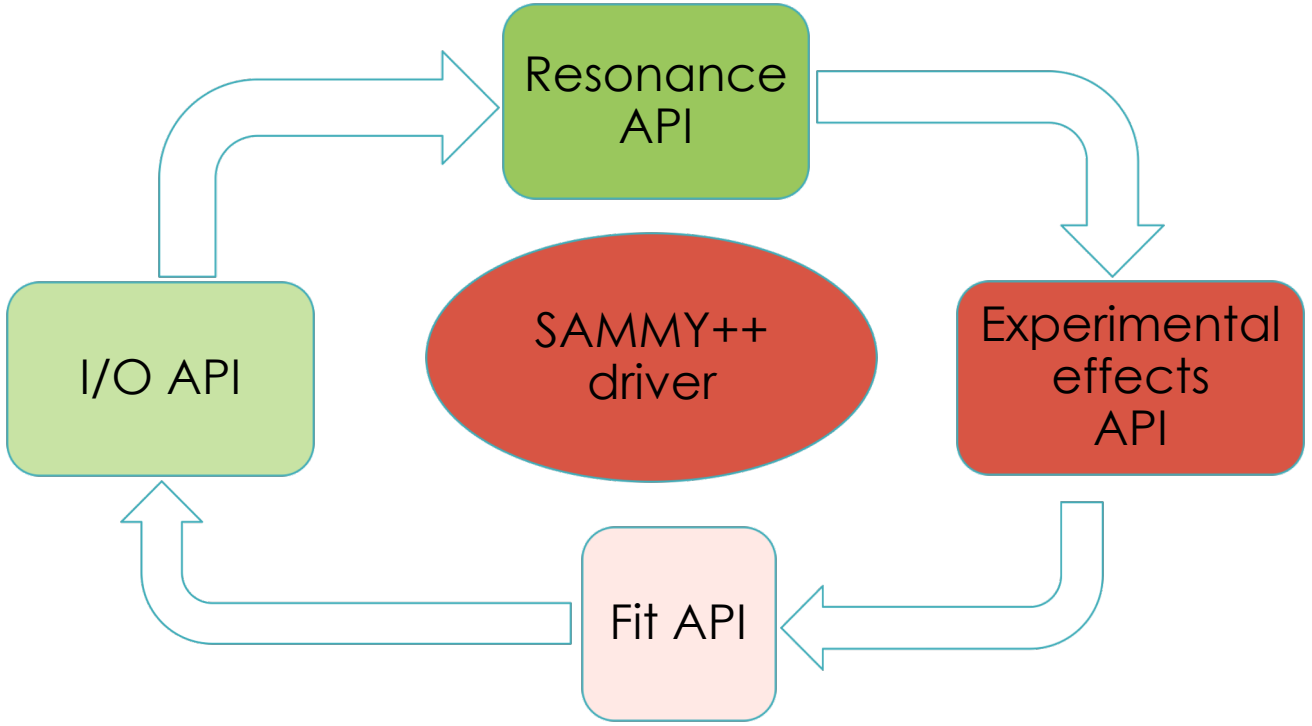
- Multilevel, multichannel R-matrix code
- Bayesian fitting of R-matrix resonance parameters (RPs)
  - Also known as generalized least squares
  - Yields covariance matrix of RPs
- Data reduction:
  - Experimental facility resolution functions: ORELA, RPI, GELINA; used for nTOF
  - Normalization, background
- Detector resolution functions: configurable for variety of detectors
- Doppler broadening: Solbrig's kernel, Leal-Hwang method
- Multiple scattering effects and other target effects
- Charged projectiles (p, α)
- Unresolved resonance range (FITACS by F. Froehner)

SAMMY features introduced in 8.1 (2017):

- SAMINT: integral benchmark experiments inform research parameter evaluations (V. Sobes, L. Leal, G. Arbanas, https://info.ornl.gov/sites/publications/Files/Pub50343.pdf)
- SAMMY was integrated into SCALE software quality assurance (SQA) in AMPX footsteps
  - Automated cmake/ctest suite, revision control repository, FogBugz
  - Platforms supported: Linux/gfortran, Mac/gfortran, Windows/ifort
- New detector resolution functions were developed in collaboration with Rensselaer Polytechnic Institute (RPI)
- Updated physical constants, which are identical in SAMMY and SAMRML
- Implemented several other bug fixes and added 6 test cases

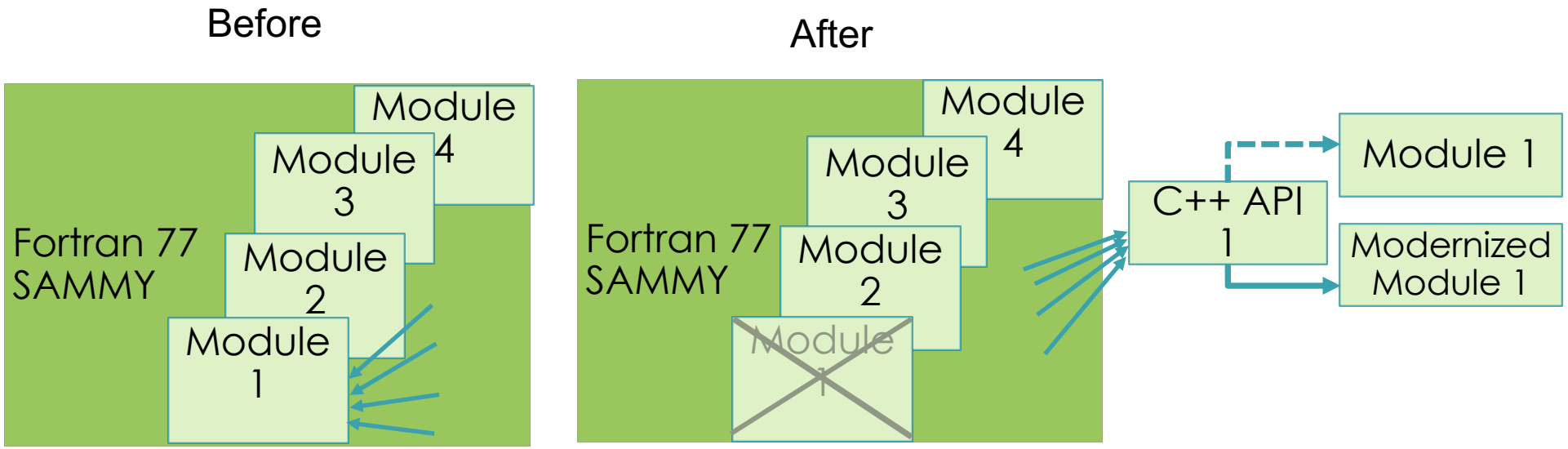
SAMMY++ high-level application programming interface (API)

- Defines APIs before implementation
  - Enables interchangeable implementations for each API
  - Leverages input/output (I/O) and resonance API in modernized AMPX
    - SAMMY parameter and GND file reader/writer under development
    - Will replace SAMMY I/O routines



Modular modernization of SAMMY using APIs

Schematic diagram of SAMMY Fortran 77 legacy module modernization



Example: modernization of Coulomb functions

- **Background:** Coulomb functions are used in SAMMY to compute the R-matrix Shift and Penetrability functions needed to compute cross sections for charged-particle projectiles
- **Problem:** Shift functions are needed at negative energies for evaluations spanning channel thresholds but cannot be computed by SAMMY
- **Solution:** Coulomb functions will be modernized via the C++ API method outlined on the previous slide:

  (Leverage modern C++ Coulomb functions published by N. Michel 10.1016/j.cpc.2006.10.004
- **Issues:** 3 variants of Coulomb, Shift, and Penetrability functions are called in the legacy SAMMY depending on the values of input parameters; negotiated an Oak Ridge National Laboratory (ORNL) lab-wide license for use and distribution of Coulomb functions
- **Benefit:** Enables inclusion of channels below their thresholds (next); enables conversion from R-matrix parameters to (and from) the Brune's alternative R-matrix, or the S-matrix poles, also known as Hwang "multipole" representations

Example: modernization of Coulomb functions

- Code sharing of Coulomb functions with AMPX/SCALE
- N. Michel, "Precise Coulomb wave functions for a wide range of complex ℓ, η and z", Computer Physics Communications, Volume 176, Issue 3, 1 February 2007, Pages 232-249, http://doi.org/10.1016/j.cpc.2006.10.004.
- Several test cases re-baselined with more accurate solutions
- NEW test case added for Coulomb functions using high precision tabulated values
- Analytical simplifications for eta >> rho were retained to avoid numerical difficulties
- Analytical expressions for derivatives of the R-matrix shift function, penetrability, and the phase shift for charged particles have been implemented for the first time in SAMMY
  - Previously computed numerically for charged particles,
  - already computed analytically for neutrons

Replacing COMMON blocks by F90 MODULES

- Few weeks of concentrated efforts by Wiarda, Holcomb, Arbanas, Chapman
- On the order of ~100 COMMON blocks in separate files
  - Each common block could have up to ~100 variables or arrays
  - Each subroutine INCLUDEs several of these files
- Replaced each COMMON block file by a corresponding F90 module
- In-house Perl Script to globally replace each INCLUDE by a USE module statement
- SAMMY test cases re-run after global replace for each file
  - Any failing tests would then be resolved
  - The last few particularly difficult ones were resolved by Doro
- All COMMON block replaced and all test cases passing

Modernization of SAMMY methods

- **Background:** Nuclear theories, measured data, and optimization methods are becoming more sophisticated
- **Problem:** Although SAMMY is robust, its methods must advance
- **Solution:** Conceptual advances in evaluations methods are needed for cross section models and data optimization methods
- **Benefits:** Conceptual advances pave the way for advanced functionality

Simultaneous evaluations of thermal and resolved resonance region (RRR)

Bayesian optimization of defective models and incomplete data covariances (GLS and MC)

Generalized Reich-Moore approximation and its Brune transform; direct capture

Simultaneous evaluation of S(α,β) and RRR

- **Problem:** S(α,β) and RRR are evaluated *separately* by different evaluators/codes
  - Covariance between the two is absent; may lead to discontinuity at the interface
  - Caused by distinct physical theories and codes used in respective evaluations
- **Solution:**
  - Developed S(α,β) expertise (C. Chapman) and couple with RRR expertise at ORNL
  - Relate parameters in S(α,β) and RRR and evaluate simultaneously
  - Coding is required to interface the optimization code to the S(α,β) and RRR codes
- **Benefits:**
  - Consistent evaluations of S(α,β) and RRR, including cross-covariances
  - Thermal S(α,β) cross sections include T-effects cf. conventional Doppler broadening
  - Similar problems exist at the interface of RRR and URR

Scattering length for S(α,β) and RRR

- This expression relates the bound scattering length used in S(α,β) evaluations to SAMMY RRR R-matrix parameters

$$b(E) = \frac{A+1}{A} a(E)$$

$$a(E) = a_{s\text{-wave}}(1 - R_\infty - \frac{\gamma_{1s}^2}{E_1 - E - i\Gamma_{1\gamma}/2 - ik\gamma_{1s}^2})$$

- Complex scattering lengths model thermal neutron absorption
  - Complex R-matrix channel radius to model direct capture introduced on the next slide
- Also, SAMMY module DOPUSHx computes crystal lattice effects on low energy resonances
  - Naberejnev (1999)

Direct capture parameterization by complex channel radii

- Motivated by an expression for thermal neutron capture cross section

$$\lim_{E\to 0^+} \sigma_\gamma(E) = \frac{4\pi}{k} b_i(E) = \frac{4\pi}{k}\left(\frac{A+1}{A}\right) a_i(E)$$

- Where

$$\begin{aligned} a(E) &= a_0(1-\mathcal{R}(E)) \\ &= a_r(E) - \imath a_i(E) \\ a_0 &= a_{0r} - \imath a_{0i} \end{aligned}$$

S-wave (complex!) R-matrix channel radius

$$\begin{aligned} \mathcal{R}(E) &\equiv \sum_\lambda \frac{\gamma_{\lambda s}^2}{E_\lambda - E - i\Gamma_{r\gamma}/2 - ik\gamma_{\lambda s}^2} \\ &= \mathcal{R}_r(E) + i\mathcal{R}_i(E) \end{aligned}$$

- It follows: $a_i(E) = a_{0r}\mathcal{R}_i(E) + a_{0i}(1-\mathcal{R}_r(E))$; interference in the last term!

Direct capture (DC) parameterization by complex channel radii

- Unitarity is still enforced as in the Reich-Moore Approximation:
  - Direct *and* resonant capture channels are now eliminated together
  - Total cross section = (total *capture* cross section) + (total *particle* channel cross section)
    = (*eliminated channels*) + (*retained channels*)
  - Unitarity of the total scattering matrix (including eliminated capture) is enforced exactly
- Provides a simple phenomenological R-matrix parameterization of DC
  - Works for conventional or generalized Reich-Moore approximation
  - Alternative to physical modeling of direct capture, e.g. single-particle potential model:
    - No need for energies or spectroscopic factors of capturing bound states
  - Could be encoded by a straightforward extension of the current ENDF format
- Can be applied to:
  - *Westcott factors:* an integral measure of deviation of thermal capture c.s. from ~1/k
  - *Interference effects:* estimated by Raman and Lynn for thermal neutron capture as:

$$\sigma_\gamma(\mathbf{X}) = (\sigma_{\mathrm{dir},\gamma}^{1/2} \pm \sigma_{\mathrm{CN},\gamma}^{1/2})^2$$

Thermal *scattering* cross sections at 0 K with complex radii

- High precision measurements of thermal neutron capture *and* scattering data provide useful constraints on (complex) R-matrix channel radii and resonance parameters
- Contribution from loosely bound resonances may affect thermal c.s.
  - A single loosely bound narrow resonance conventionally added to fit thermal c.s. data
- Phenomenological R-matrix formalism can accommodate complex channel radii by analytical continuation
  - To parameterize direct capture at all energies, and for `l>0` capture channels
  - N.B. Imaginary part of R-matrix channel radius could exhibit slow variation with energy

$$\lim_{E\to 0^+} \sigma_s(E) = \frac{4\pi}{k}|b(E)|^2 = \frac{4\pi}{k}\left(\frac{A+1}{A}\right)^2 |a(E)|^2$$

$$|a(E)|^2 = |a_0|^2|1-\mathcal{R}(E)|^2$$

Bayesian optimization of *defective* models

- **Background:** Bayes theorem takes ***prior*** information:
  - model parameters AND
  - measured data

  and yields ***posterior*** probability distribution functions of parameters *and* data
  - model parameters AND
  - measured data
- **Problem:** Bayes theorem assumes
  - perfect *model* AND
  - perfect *covariances*

  ➡ violation of either one yields incorrect posterior values or unreasonably small uncertainties
- **Two pronged solution:**
  - Formally introduce model defect into the Bayes' theorem (cf. Georg Schnabel's Ph.D. Thesis, 2015)
  - Introduce scaling of chi^2 in the Bayesian MC weight to yield expected number of DOF
- **Benefits:**
  - Intuitive generalization of Bayesian theorem for model defects
    - posterior data values are no longer forced to equal posterior model prediction

Bayesian optimization of generalized data for *defective* models

- Expressed as a conventional minimization of the cost function (chi^2)
  - G. Arbanas et al., CW2017; overlap with Schnabel (Ph.D. Thesis, TTU, Vienna, 2015)

Cost function (a.k.a. chi^2):

$$Q(z) \equiv (z - \langle z \rangle)^\intercal \mathbf{C}^{-1} (z - \langle z \rangle)$$

Constraint:

$$T(P) - D = \delta$$

where generalized data includes defect:

$$z \equiv (P, D, \delta)$$

$$\langle z \rangle \equiv (\langle P \rangle, \langle D \rangle, \langle \delta \rangle)$$

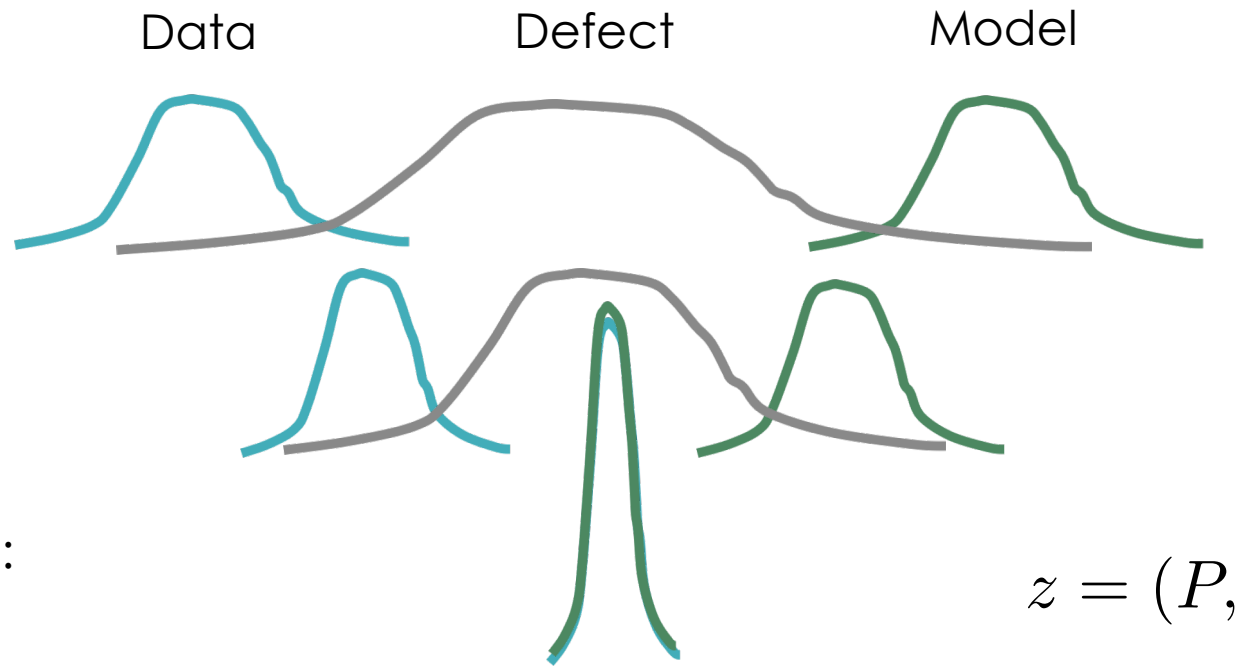
$$\mathbf{C} \equiv \langle (z - \langle z \rangle)(z - \langle z \rangle)^\intercal \rangle \equiv \begin{pmatrix} \mathbf{M} & \mathbf{W} & \mathbf{X} \\ \mathbf{W}^\intercal & \mathbf{V} & \mathbf{Y} \\ \mathbf{X}^\intercal & \mathbf{Y}^\intercal & \mathbf{\Delta} \end{pmatrix}$$

Inclusion of model defect increases posterior uncertainties

$$(z-\langle z\rangle)^{\intercal}\mathbf{C}^{-1}(z-\langle z\rangle)$$

$$z \equiv (P, D, \delta)$$

$$T(P) - D = \delta$$



$$z = (P, D)$$

$$T(P) = P$$

Impact of PRIOR covariances: Generalized Least Squares (GLS)

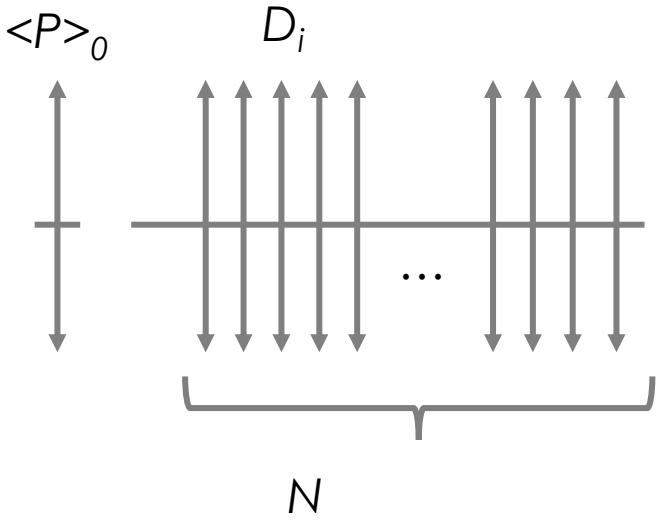
- GLS via e.g. Newton-Raphson Method
- Unaccounted correlations in data yield uncertainties that are too small

$$z = (P, D) \qquad T(P) = P$$

$$(z - \langle z \rangle)^{\intercal} \mathbf{C}^{-1} (z - \langle z \rangle)$$

$$\mathbf{C_0} = \begin{pmatrix} m_0 & w_0 \\ w_0 & v_0 \end{pmatrix} = \begin{pmatrix} 1 & w_0 \\ w_0 & 1 \end{pmatrix}$$

$$m_N \xrightarrow[N \to \infty]{} \begin{cases} 0, & w_0 = 0 \\ 1, & w_0 = 1 \end{cases}$$



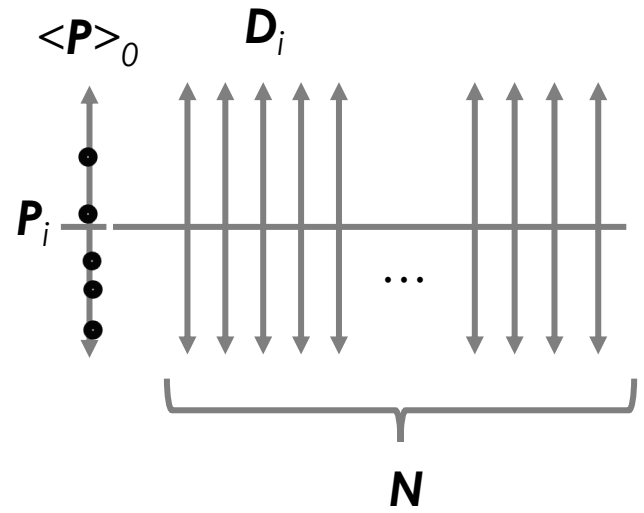
Impact of PRIOR covariances: Monte Carlo (MC)

- MC of SNS data yielded unrealistic MC weight (one dominant)
  - Posterior parameter covariance should be constrained by the number of DOFs
  - by rescaling it to yield the correct # of DOFs to correct for imperfect prior covariances

$$(z-\langle z\rangle)^{\intercal}\mathbf{C}^{-1}(z-\langle z\rangle)$$

$$\mathbf{C}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \omega_i = e^{-\chi_i^2} = e^{-N(P_i-D)^2/2}$$

$$\langle P\rangle_N \equiv \sum_i^N \omega_i P_i \xrightarrow[N\to\infty]{} \min\{P_i\} \qquad m_N \equiv \langle(\delta P)^2\rangle_N \xrightarrow[N\to\infty]{} 0$$

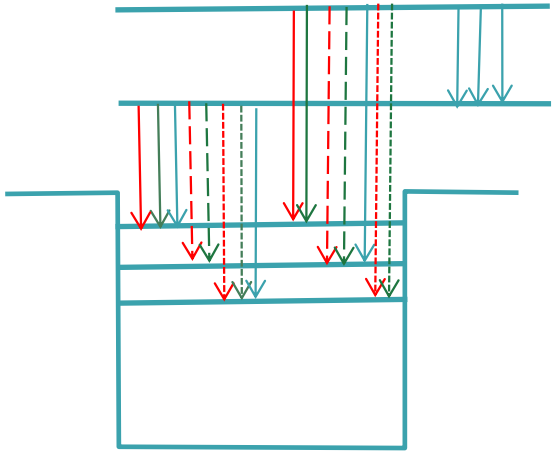


$$\mathbf{C}_0 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad \omega_i \equiv e^{-\chi^2/N} = e^{-(P_i-D)^2/2}$$

$$\langle P\rangle_N \xrightarrow[N\to\infty]{} \langle P\rangle_0 \qquad m_N \equiv \langle(\delta P)^2\rangle_N \xrightarrow[N\to\infty]{} m_0 \equiv \langle(\delta P)^2\rangle_0$$

Generalized Reich-Moore approximation

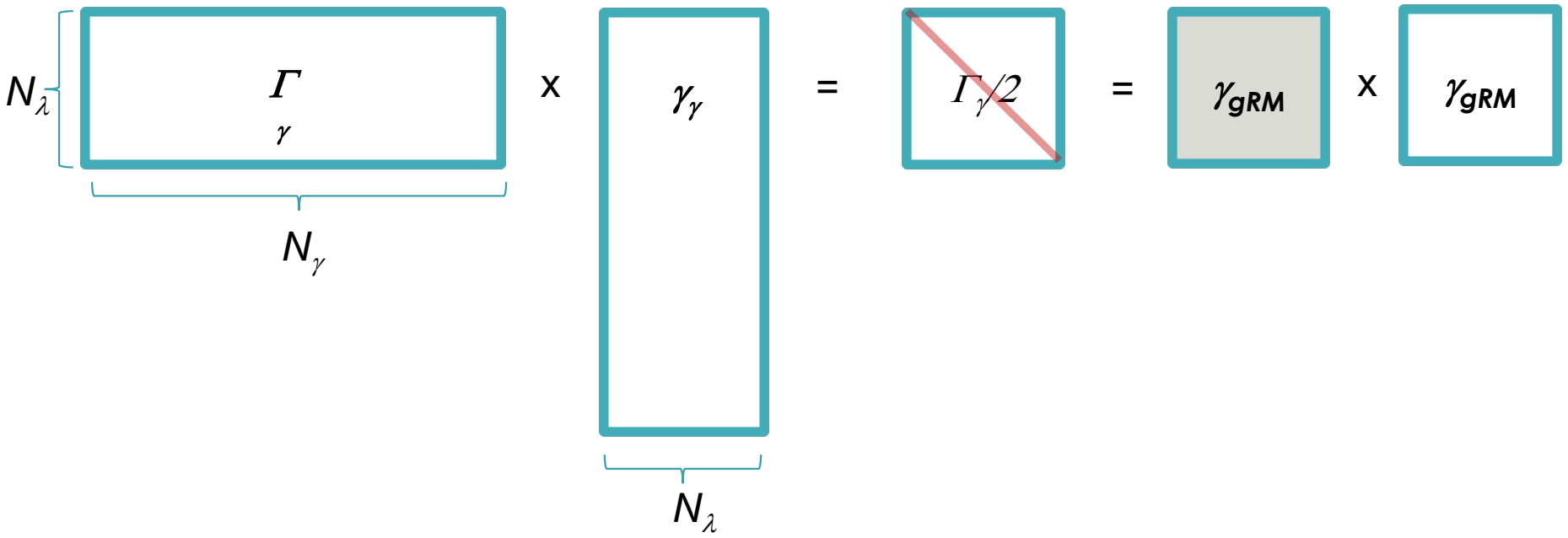
- γ-ray channels
  - Defined by EM multipolarity, helicity, and final state quantum numbers
  - Selection rules based on final state quantum numbers, γ-ray multipolarity
  - Electric: E1, E2, E3 …
  - Magnetic: M1, M2, M3 …
- Level-level interference takes place via identical γ-ray channels



G. Arbanas, V. Sobes, A. Holcomb, P. Ducru, M. Pigni, and D. Wiarda (ND2016), *EPJ Web of Conferences* **146**, 12006 (2017) https://doi.org/10.1051/epjconf/201714612006

Generalized Reich-Moore approximation

- Consider capture-width parameter matrix for $N_\lambda << N_\gamma$:



- Since total capture cross section depends on Γ_γ, it could be fit equally as well by N_λ as it could by all N_γ capture channels
  - this is true for *total* capture only
  - individual γ-channels require full *R*-matrix

Brune transform for Reich-Moore Approx. R-matrix widths

- Conventional Reich-Moore Approximation (RMA): 1 capture width per resonance
- Brune transform of RMA parameters is made possible by generalized RMA (GRMA)

$$\tilde{\gamma} = \mathbf{a}^{\mathsf{T}}\gamma$$

since $\tilde{\gamma}$ attains non-zero off-diagonal elements even when γ is diagonal

- Conventional boundary condition for capture channels ensures that the non-linear eigenvalue equation for Brune-transformed resonance widths remains unchanged

SAMMY 8.2 anticipated features in early 2019

1. Incorporate a C++ Coulomb function library CWFCOMPLEX into SAMMY/AMPX
2. Include closed channels in the SAMMY R-matrix (IAEA R-matrix collaboration)
3. Include closed channels in computation of analytical derivatives of cross sections inside SAMMY
4. Correct the bugs in the SAMMY I/O of ENDF files for charged particles by linking to the modern C++ ENDF I/O AMPX library
5. Enable conversion from Reich-Moore Approximation R-matrix parameters to Brune's alternative R-Matrix parameters
6. Update SAMMY documentation accordingly.
7. Release SAMMY under an open source license

Summary and outlook

- SAMMY 8.1 released in 2017
- SAMMY is under the SCALE SQA framework
- Modernization proceeds via API framework, including Coulomb functions, optimization…
- Code sharing with AMPX/SCALE (D. Wiarda, A. Holcomb) guarantees consistency and is conducive to new data formats
- Potential improvements to evaluation methods have been identified
  - Simultaneous evaluation of thermal and resolved resonance ranges
  - Generalized Reich-Moore approx. and direct capture via complex channel radii
  - Optimization of defective models via GLS or MC
- Open source SAMMY release is in progress, as well as AMPX
- SAMMY 8.2 is expected later in early 2019

Special thanks to SAMMY contributors

- Andrew M. Holcomb (ORNL)
- Dorothea Wiarda (ORNL)
- Marco T. Pigni (ORNL)
- Vladimir Sobes (ORNL)
- Chris W. Chapman (ORNL)
- Jesse Brown (RPI)

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Auxiliary slides

Fit API: Preliminary interface

Interface
Fit

setData
: Set an instance of Data interface

initialize
: After setting data object initialize internal data structures

execute
: Do the actual fitting

finalize
: Clean up any internal resources

Interface
Array

getNumDim
: Get the number of dimensions

getSize(int dim)
: Get the array size for dimension m

getValue(int i1, int i2, …)
: Get the value for the indicated indices. In C++ we would pass in a vector of length getNumDim

setValue(int i1,int i2, …)
: Set value

Interface
Data

getNumberParams
: Get the number of parameters

getNumData
: Get the number of experimental data

getData
: Get the list of experimental data (1-dim Array)

getParam
: Get the list of initial params (1-dim Array)

getCovMatrix
: Get the full covariance matrix (2-dim Array)

getTheory
: Get theoretical values based on current parameters (1-dim Array)

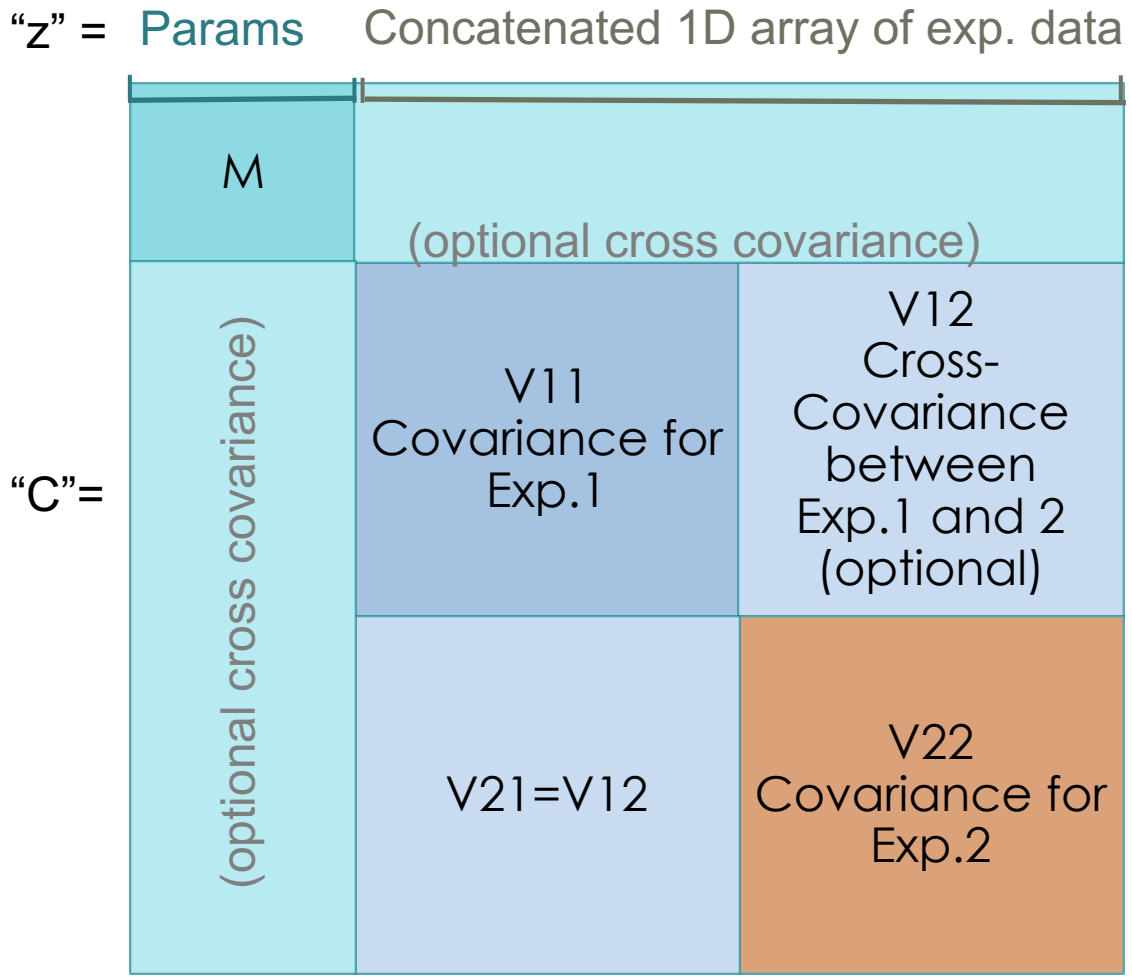
setParam
: Set the current parameters (1-dim Array)

setCovMatrix
: Set the full covariance matrix (2-dim Array)

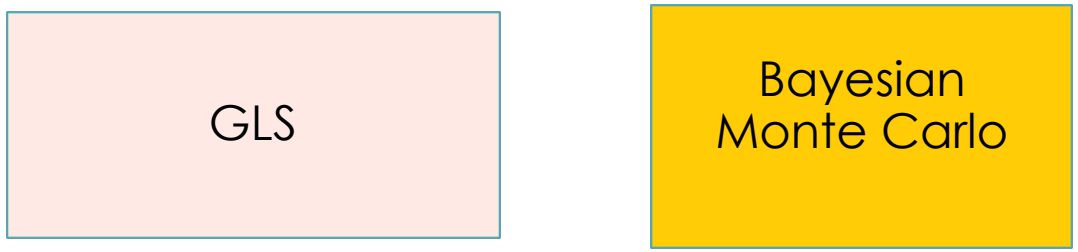
- Actual instances are instantiated by a factory class
- Data will have a method to obtain the derivatives (2-dim Array: getNumberParams x getNumData); there will be a function that computes derivatives numerically
- Fit calls setParams, getTheory, setCovMatrix repeatedly in the course of fitting the data

Fit API: GLS implementation

- Parameters and experimental data cast into 1D array by implementation of data
  - for generic use inside SCALE framework
  - Froehner's formulation and notation:



Fit API: GLS, Bayesian Monte Carlo



- Generalized least squares (GLS)
  - Nuclear Engineering Science Laboratory Synthesis (NESLS) summer intern Jinghua Feng implemented a prototype
  - Andrew Holcomb ported the prototype into the FitAPI
- Implementation uses *cpp-array* library (CPC **185**,1681, 2014)
  - Transparently parallelized via BLAS library (Intel MKL)
  - Compact expressions implemented directly (Sect. 2.2, JEFF Report 18, 2000)
- BLAS speeds up large matrix operations in SAMMY and shortens code
  - Arbanas, Dunn, Wiarda, M&C2011, http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/47/073/47073019.pdf

Experimental effects (EE) API

- Convolution of Doppler broadening, target, and detector effects, each one implenting the EE API:

- SHIFT API for on-the-fly neutron transport aspects
  - To enable fitting integral benchmark experiments (IBEs)
  - Developed for SCALE by Cihangir Celik in FY2017
  - Message passaging interface (MPI) enabled
  - Could use MCNP input
- In principle, the entire experimental setup could be simulated; fitting to raw data may be desirable to avoid PPP; varying opinions

Modular modernization of SAMMY using APIs

For each SAMMY Fortran 77 legacy module to modernize:

1. Create a layer of indirection to the module by designing its C++ API
2. Move the module out of SAMMY and use it to implement its C++ API
3. Redirect all module calls to the C++ API implementation outside SAMMY and then re-run SAMMY test cases and correct any problems until identical results are reproduced
4. Implement the C++ API using a modernized code or a third-party library
5. Recompile SAMMY with the modern implementation of the C++ API and then re-run SAMMY test cases and re-baseline the results when justified

Phenomenological Dirac R-matrix formalism

- Originally derived for calculable R-matrix, but expressed in a form that could be used for phenomenological fitting:
  PhD Thesis (2011): http://scholarworks.wmich.edu/dissertations/411
- Boundary condition is determined by the channel radius
- Compare to approximations and the nonrelativistic R-matrix

J. Grineviciute and Dean Halderson, *Physical Review C*, **85,** 054617 (2012)

$$R_{cc'} = \sum_{\mu} \gamma_{\mu c}\gamma_{\mu c'}/(E_\mu - E)$$

$$\mathbf{S} = \mathbf{v}^{1/2}(\mathbf{Fo} - \mathbf{RGo})^{-1}(\mathbf{F_I} - \mathbf{RG_I})\mathbf{v}^{-1/2} \qquad T_{cc'} = i(\delta_{cc'} - S_{cc'})/2$$

$$\langle f\rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A} = \frac{1}{k}\sum \sqrt{4\pi(2\ell+1)} C^{\ell 1/2 j}_{0\sigma m} C^{J_A j J_B}_{M_A m M_B} C^{J'_A j' J_B}_{M'_A m' M_B} C^{\ell' 1/2 j'}_{m'_\ell \sigma m'}$$

$$\times i^{(\ell-\ell')} e^{i(\delta'_\kappa + \delta'_{\kappa'})} T_{\alpha J_A \ell j J_B,\alpha' J'_A \ell' j' J'_B} Y_{\ell' m'_\ell}(\boldsymbol{k}').$$

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{2(2J_A+1)} \sum_{\sigma\sigma' M'_A M'_A} \left| \langle f_c\rangle_{\sigma\sigma'} \delta_{J_A\alpha M_A, J'_A\alpha' M'_A} + \langle f\rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A} \right|^2$$

ORNL S(α,β) evaluation framework overview

- The objective is to combine experimental double differential scattering data and model parameters to yield the best estimate of double differential cross section (DDCS) and ***uncertainties***
- Data and simulation fit is achieved using the unified Monte Carlo (UMC) method
- Simulations are constrained by physical properties of material
- Framework is tested on light water
  - Data collected from ORNL SNS
  - Rensselaer Polytechnic Institute (RPI) collaboration
- Validated using benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook
- C. Chapman's Ph.D. https://smartech.gatech.edu/handle/1853/58693